NASA Contractor Report 3384

Zero-Gravity Aerosol Behavior

Harry W. Edwards

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I. Introduction

An orbiting laboratory provides the unusual scientific opportunity to carry out experiments in the absence of gravitational effects. Potential benefits in the field of aerosol science are the absence of sedimentation and convection. In an experiment carried out under terrestrial conditions, sedimentation is important for larger areosol particles. Preventing spurious convective currents is often troublesome in terrestrial aerosol experiments. In addition to these potential benefits, the absence of a gravitational field may provide theoretical simplification. The feasibility of an orbital aerosol experiment is therefore of scientific interest. This preliminary investigation was undertaken to examine the feasibility and scientific benefits for a zero-gravity aerosol behavior experiment in an orbiting laboratory.

II. Objectives

A. Examine the theoretical feasibility for a zero-gravity aerosol behavior experiment.

B. Examine the technological feasibility for a zero-gravity aerosol behavior experiment.

C. Identify potential scientific benefits for the experiment.

D. Present conclusions.

III. Theoretical Feasibility

In the evaluation of experiments concerned with the disappearance of particles from a confined aerosol, one must in general consider the simultaneous concentration changes due to coagulation, diffusion, and sedimentation. The mathematical complexity of this problem has frustrated attempts to devise totally satisfactory analytical models, even for initially monodisperse particles in the absence of electrostatic and convective effects. The conduct of such experiments under the essentially zero-gravity conditions of an orbiting space laboratory would provide data in the absence of sedimentation, normally an important depletion mechanism for particles larger than a few tenths of one micrometer in radius. A key issue is whether the absence of sedimentation results in a significant reduction in the mathematical complexity of the problem.

Considerable success has been achieved in describing the behavior of dilute aerosols in which effects due to coagulation are absent. For the one-dimensional problem, the following partial differential equation giving the numerical particle concentration n as a function of time t and vertical position z has been solved analytically by Davies (1) and verified experimentally by Richardson and Wooding (2):

$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial z^2} - v \frac{\partial n}{\partial z} \tag{1}$$

The aerosol considered by these investigators was monodisperse and confined between perfectly absorbing parallel surfaces of large horizontal extension such that effects due to the vertical walls were negligible. The particle diffusion coefficient D and settling velocity v may be evaluated from theoretical considerations given by Fuchs (3).

A major problem associated with achieving a general solution which includes coagulation is the evolution of the particle size distribution with time. Hidy and Brock (4) reviewed many investigations of coagulation and found that the only exact solution is due to Smoluchowski (5) in which the coagulation constant is independent of time. In the absence of particle depletion due to diffusion and sedimentation, the basic equation of coagulation is

$$\frac{dn}{dt} = -Kn^2 \tag{2}$$

where K is 8πRD for spherical particles of radius R. Integration of equation (2) gives

$$\frac{1}{n} - \frac{1}{n_o} = Kt \quad \text{or} \quad \frac{n}{n_o} = \frac{1}{1 + n_o Kt} \tag{3}$$

where n_o is the initial particle concentration at t = 0. Numerous experimental studies reviewed by Fuchs (3) establish the linear relationship between n^{-1} and time although values for K tend to be somewhat larger than computed values. Hidy and Brock (4) suggested that the lack of quantitative agreement is attributable to electrical effects, spurious air currents, increasing polydispersion, and the need for a slip correction. The effect of increasing polydispersion was investigated by Hidy (6) who numerically solved a set of simultaneous nonlinear differential equations for a discrete particle size distribution. The numerical results give values for n(t) which closely match those given by equation (3), although changes in the relative concentrations in individual particle size categories differ from those for constant particle collision parameter. Various authors have suggested that the increase in mean particle size to decrease K is offset by the increasing polydispersion with its opposite effect. The linear relationship between n^{-1} and time is used in the present work to develop a macroscopic model for the combined effects of diffusion and coagulation.

The equation for the general case which includes coagulation gives n(x,y,z,t) by

$$\frac{\partial n}{\partial t} = D \nabla^2 n - v \frac{\partial n}{\partial z} - Kn^2 \qquad (4)$$

where $\underline{D}$, $\underline{v}$, and $\underline{K}$ are assumed independent of time and position. The assumptions of perfectly absorbing walls and uniform initial particle concentration $\underline{n_o}$ give $n(x,y,z,t) = 0$ at the walls and $n(x,y,z,0) = n_o$ in the chamber. Equation (4) has been solved analytically by Wilhelm (7) for the mathematically similar problem of contained plasma particles undergoing simultaneous recombination, diffusion, and convection. Wilhelm's approach, which involves a transformation to a differential equation in which the nonlinear term becomes a small perturbation, was shown to apply to plasma particles confined by nonreflecting walls. Application to the coagulating aerosol undergoing simultaneous depletion by diffusive deposition was made by Benedict (8). The details of this treatment are given in Appendix I.

The theoretical feasibility for a zero-gravity aerosol study was examined by carrying out simulated experiments with models developed by Benedict (8). The purpose of the computations was to determine whether the requirements for a zero-gravity aerosol study are, at least in principle, compatible with the time and space limitations for an orbital experiment. Input to the models consists of the particle properties and initial concentration, gas properties, and chamber geometry. Output consists of the particle concentration as a function of time and location in the chamber. Numerical results are given in Appendix I.

Two conclusions arise from the theoretical feasibility study. Firstly, the time and physical space limitations for an orbital experiment are not prohibitive in terms of obtaining kinetic data.

For example, experiments of a duration of 1-2 hours in a cylindrical chamber ($r = 25$ cm, $h = 50$ cm) can produce meaningful data on the history of the aerosol confined in the absence of gravitational effects. Secondly, the model is internally consistent and produces physically reasonable results.

While the solution procedure resulted in substantial simplification of the problem, the reduction in complexity is only partly attributable to the absence of the gravitational term. The nonlinear coagulation term necessitates a transformation of variables, whether or not the gravitational term is present.

A final point concerns possible limitations of the models employed in the theoretical analysis. Both $\underline{D}$ and $\underline{K}$ have been used as ensemble parameters. The major limitation of this approach is that the models do not provide direct information on the evolution of the particle size distribution. It should also be emphasized that while equation (1) has been verified experimentally, equation (4) must still be regarded as a postulate. The experimental conditions under which it is permissable to treat both $\underline{D}$ and $\underline{K}$ as ensemble parameters in equation (4) are considered in Appendix I.

IV. Technological Feasibility

The technological feasibility was examined by addressing the following issues:

A. Experiment Definition

B. Requirements for Aerosol Generation

C. Requirements for Measuring Particle Concentrations

D. Requirements for Data Analysis

The major findings are summarized in a previous report (9). Two areas of concern have been identified. The first is the current absence of a single, totally satisfactory experimental technique for determining aerosol particle concentrations over the particle size range of 10^{-7} cm to 10^{-3} cm. Either complementary experimental techniques would be required or, alternatively, the size range accessible must be narrowed to be compatible with a single experimental technique. In view of the potential problems associated with calibration of complementary techniques under orbital conditions, the latter alternative seems more practical.

The second area of concern is that of determining the particle concentration to the accuracy required. For example, in the absence of electrostatic and convective effects, calculated and measured values of the coagulation constant $\underline{K}$ differ by perhaps 10%. Clearly, the experimental technique selected must be capable of resolving differences in particle concentrations smaller than 10% in order to make meaningful comparisons between experimental and theoretical data. While considerable progress has been made in recent years in refining experimental methodologies in aerosol science, the required accuracy may not be available for the ranges of particle sizes and concentrations of interest. However, recent developments with electrostatic classifiers and light-scattering techniques are particularly encouraging. The required instrumental capabilities may not be far away, but the situation seems borderline at this time.

V. Scientific Benefits

Potential scientific benefits of a zero-gravity aerosol study include validation of theoretical models for aerosol kinetics and measurement of $\underline{D}$ and $\underline{K}$ in the absence of convective effects. However, because of existing gaps in both the theoretical and experimental aspects, such an experiment would probably be premature at this time. In order for the potential benefits to be fully realized, more detailed theoretical models for the combined effects of coagulation and diffusion are needed. Moreover, additional refinements in certain experimental methodologies would be helpful to assure accurate measurements over the ranges of particle sizes and concentrations of interest.

VI. Conclusions

The theoretical feasibility for a zero-gravity aerosol study has been examined. The mathematical complexity of the problem is discouraging if one attempts to retain a detailed picture of the combined effects of coagulation and diffusion upon the evolving particle size distribution. However, an analytical solution is possible if one considers only the particle concentration $\underline{n}$ and treats $\underline{D}$ and $\underline{K}$ as ensemble parameters. Experimental studies support use of $\underline{K}$ as an ensemble parameter in many cases. Treating $\underline{D}$ as an ensemble parameter imposes some limitations, however. The results of the macroscopic treatment show that an aerosol decay experiment is feasible in a compact chamber for a time duration of the order of hours. It is concluded that the limitations of physical space and time for an orbital experiment are not prohibitive in terms of conducting an aerosol experiment.

Because of the present mathematical difficulties associated with treating the combined effects of coagulation and diffusion, reservations are expressed about the scientific urgency for a zero-gravity aerosol study at this time. The experiment would also appear to stretch existing capabilities for characterization of aerosol particles. Nevertheless, the need for reliable and accurate aerosol behavior data in the absence of convective effects is recognized. Periodic re-examination of the need for a zero-gravity aerosol study is therefore recommended. When such a study is planned, it will be important to include a complementary terrestrial investigation. The difficulties associated with carrying out an experimental aerosol study under favorable terrestrial laboratory conditions can be formidable. The success of an orbital experiment will be highly dependent upon managing these difficulties and anticipating additional problems posed by the orbital situation.

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Appendix I

THESIS

THEORETICAL BEHAVIOR OF A CONFINED AEROSOL

Submitted by

Bruce John Benedict

In partial fulfillment of the requirements
for the Degree of Master of Science
Colorado State University
Fort Collins, Colorado
Fall, 1977

COLORADO STATE UNIVERSITY

Fall, 1977

WE HEREBY RECOMMEND THAT THE THESIS PREPARED UNDER OUR SUPERVISION BY BRUCE JOHN BENEDICT ENTITLED THEORETICAL BEHAVIOR OF A CONFINED AEROSOL BE ACCEPTED AS FULFILLING IN PART REQUIREMENTS FOR THE DEGREE OF MASTER OF SCIENCE.

Committee on Graduate Work

Adviser

ABSTRACT OF THESIS

THEORETICAL BEHAVIOR OF A CONFINED AEROSOL

Coagulation, sedimentation and diffusive deposition are the primary removal mechanisms for an aerosol confined in a chamber on earth. The equation describing the depletion rate due to these mechanisms is a second order nonlinear partial differential equation. For an aerosol in a zero-gravity environment the sedimentation term drops out, but this does not change the basic nature of the equation. An analytical solution to the resulting equation is presented and particle concentrations are computed as a function of time and location in a cylindrical chamber.

The equation is also solved for an aerosol under the influence of a gravitational field. There are some difficulties with this solution where the removal mechanisms are operating at similar rates. These are overcome by modelling the decay process as if diffusion were not present. Results of the two models indicate that sedimentation is the most important of the removal mechanisms. Coagulation is next in importance and diffusion is negligible except within 1 centimeter of the chamber wall.

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NOMENCLATURE

A	Constant in mobility equation
A_{ij}	Fourier coefficients for solution
b	Constant in mobility equation
B	Particle mobility
C	Cunningham slip Correction
C_d	Particle drag coefficient
f	Variable to which u is transformed
g	Acceleration of gravity
H	Height of chamber
i	Index for eigenvalues associated with J_o
j	Index for eigenvalues associated with sine
J_o	Zero order Bessel function
J_1	First order Bessel function
k	Boltzmann's constant
K	Particle coagulation coefficient
L	Dimensionless chamber height
n	Numerical concentration of particles
n'	Dimensionless concentration
n_o	Initial concentration of particles
Q	Constant in mobility equation
r	Radial coordinate
r'	Dimensionless radial coordinate

NOMENCLATURE (cont')

R	Particle radius
R^*	Chamber radius
R_e	Particle Reynolds number
$s(x)$	Unit step function
t	Time
t'	Dimensionless time
u	Variable to which n is transformed
U_r	Function of r' only used in separation of variables
U_z	Function of z' only used in separation of variables
U_t	Function of t' only used in separation of variables
v	Terminal settling velocity of particle
V	Particle velocity before applying Cunningham slip correction
x'	Distance from wall
z	Vertical coordinate
z'	Dimensionless vertical coordinate
β	Dimensionless coefficient
γ	Dimensionless coefficient
δ	Mean free path of air molecules
ε	Perturbation on diffusion
ν	First separation constant
σ	Second separation constant
λ_i	Eigenvalue associated with J_o
ρ	Density of air
ρ_p	Density of particle
μ	viscosity of air

CHAPTER I

EQUATION

Introduction

The principal removal mechanisms for an aerosol confined in a chamber which is located in a gravitational field are sedimentation, coagulation, and diffusive deposition at the wall. In most situations of interest sedimentation is the most important. An experiment carried out in the zero-gravity environment of an orbiting space craft would provide a unique opportunity to study aerosols. By placing an aerosol in such an environment it is possible to obtain measurements of the coagulation coefficient and diffusion coefficient of the particles. This study provides a model with which such an experiment can be designed. A model which describes the depletion of an aerosol stored in a gravitational field is also presented.

For the purposes of this modelling effort the following assumptions were made: 1. The particles are unit density spheres. 2. The system is monodisperse. 3. Initially, the particles are uniformly distributed within the chamber. 4. The coagulation coefficient is constant with respect to time. The particle formed when two particles stick together should have a coagulation coefficient which is larger than that of a single particle because the combined particle is larger. However, Fuchs [1] states that this effect is almost balanced by the decreased diffusivity of the larger particle. 5. All collisions, particle-particle and particle-wall, have a sticking coefficient of unity. Fuchs [1] indicates that as long as the only driving forces in the system are thermal, the sticking coefficient is nearly one.

Equation

Richardson and Wooding [2] present an equation describing the depletion of a monodisperse aerosol which is confined in a chamber in a gravitational field.

$$\frac{\partial n}{\partial t} = D\nabla^2 n - v\frac{\partial n}{\partial z} - Kn^2 \tag{1}$$

where n is the numerical concentration of particles, t is time, D is the particle diffusion coefficient, v is the terminal settling velocity of the particle, z is the vertical coordinate of the chamber, and K is the particle coagulation coefficient. The boundary conditions are implicit in the assumptions. Because the sticking coefficient for particles colliding with walls is unity, a particle which strikes a wall sticks to it and is thus removed from the bulk of the chamber. Thus we have $n(r,z,t) = 0$ at the walls. The initial concentration was assumed to be uniform throughout the chamber, thus the initial condition is $n(r,z,0) = n_o$.

Coefficients

Strauss [3] gives a procedure for calculating the terminal settling velocity for aerosol particles in terms of the particle Reynolds number, R_e, and the particle drag coefficient, C_d. The procedure is to first calculate the product, $C_d R_e^2$, using properties of the particles and the fluid in which they are dispersed.

$$C_d R_e^2 = \frac{32\rho(\rho_p - \rho)R^2 g}{3\mu^2} \qquad (2)$$

where ρ is the fluid density, ρ_p is the particle density, g is the acceleration of gravity, R is the particle radius and μ is the viscosity of air. Davies [4] gives a series of empirical formulas for the Reynolds number in terms of the product $C_d R_e^2$. Once the Reynolds number is determined the product can be used to find a value for the drag coefficient. These values are then used in Stokes law to find a velocity, V,

$$V = \frac{16R\rho g(\rho_p - \rho)}{3C_d R_e \mu} \qquad (3)$$

The terminal settling velocity is determined from V by applying the Cunningham slip correction,

$$C = 1 + \frac{\delta}{R}(1.257 + 0.400\exp(-1.10\frac{R}{\delta})) \qquad (4)$$

where C is the Cunningham slip correction, δ is the mean free path of the fluid molecules. Now it is possible to determine a value for the terminal settling velocity, v.

$$v = CV \qquad (5)$$

The diffusion coefficient is given in Fuchs [1]

$$D = kTB \qquad (6)$$

where k is Boltzmann's constant, T is absolute temperature, and B is the particle mobility also given by Fuchs [1].

$$B = \frac{1 + A\frac{\delta}{R} + Q\frac{\delta}{R}\exp\left(\frac{-bR}{\delta}\right)}{6\pi R\mu} \tag{7}$$

The constants A, Q, and b are given in Millikan [5] for oil drops in air at 23C and 1 atmosphere. They are A = 0.864, Q = 0.290, and b = 1.25.

The coagulation coefficient is in Fuchs [1] as follows:

$$K = 8\pi RD \tag{8}$$

Solution

The nondimensional variables, $r' = r/R^*$, $z' = z/R^*$, $n' = n/n_o$, and $t' = tD/R^{*2}$ are introduced. R^* is the radius of the chamber. Substituting these into equation (1) results in

$$\frac{\partial n'}{\partial t'} = \nabla^2 n' - \beta\frac{\partial n'}{\partial z'} - \gamma n'^2 \tag{9}$$

where

$$\beta = \frac{R^* v}{D} \qquad \gamma = \frac{R^{*2} K n_o}{D} \tag{10}$$

The boundary conditions become $n'(r',z',t') = 0$ at the walls and the initial condition is $n'(r',z',0) = 1$.

The nonlinear coagulation term in equation (9) presents the greatest difficulty in obtaining a solution thus it is desirable to remove it using a transformation. This is done by using the solution of the Smoluchowski coagulation equation as was done by Wilhelm [6]. The transformation used was

$$n'(r',z',t') = \frac{u(r',z',t')}{1 + \gamma t' u(r',z',t')} \tag{11}$$

This results in the equation

$$\frac{\partial u}{\partial t'} = \nabla^2 u - \beta \frac{\partial u}{\partial z'} - \varepsilon \tag{12}$$

where

$$\varepsilon = \frac{2\gamma t'}{1 + \gamma t' u}\left(\left(\frac{\partial u}{\partial r'}\right)^2 + \left(\frac{\partial u}{\partial z'}\right)^2\right) \tag{13}$$

The boundary conditions remain the same for the transformed variable, u, as for the variable, n. That is $u(r',z',t') = 0$ at the walls and $u(r',z',0) = 1$.

The times of 1 and 2 hours, which are used in the calculations, are very short as compared to the characteristic time for diffusion. This is born out by the values of t', which range from 7.0×10^{-8} for large particles to 1.7×10^{-3} for small particles. The values of γ are relatively large, ranging from 15 for small particles to 1.6×10^{6} for large particles. However, the values are such that for a given particle the product $\gamma t'$ is of order 1 or smaller. It is further anticipated that except near the walls the spatial derivatives will be small. Thus the value for ε will be small.

Equation (12) can now be solved by a successive approximation technique. To do this ε is set equal to 0 and equation (12) is solved.

This is the zeroth approximation. Using the solution for the zeroth approximation a value can be calculated for ε. This value is then put back into equation (12) as a constant and the equation is solved, resulting in the first approximation. This process is repeated using the value of ε calculated from the previous approximation until the desired accuracy is obtained.

CHAPTER II

ZERO-GRAVITY SOLUTION

Equation

The simplest case for obtaining a solution is the zero-gravity situation. This is because with zero-gravity the terminal settling velocity of the particle is zero, thus $\beta = 0$ and equation (12) reduces to

$$\frac{\partial u}{\partial t'} = \nabla^2 u - \varepsilon \qquad (14)$$

Setting $\varepsilon = 0$ for the zeroth approximation results in the diffusion equation which for a cylindrical chamber is

$$\frac{\partial u}{\partial t'} = \frac{1}{r'}\frac{\partial u}{\partial r'} + \frac{\partial^2 u}{\partial r'^2} + \frac{\partial^2 u}{\partial z'^2} \qquad (15)$$

Solution

The solution for equation (15) can be found using the technique of Separation of Variables as given by Wylie [7]. For this it is assumed that the solution is the product of three functions, a function of r' only, a function of z' only, and a function of t' only. Thus

$$u(r',z',t') = U_r(r')U_z(z')U_t(t') \tag{16}$$

Substituting this into equation (15) gives

$$\frac{\frac{\partial U_t}{\partial t'}}{U_t} = \frac{1}{r'}\frac{\frac{\partial U_r}{\partial r'}}{U_r} + \frac{\frac{\partial^2 U_r}{\partial r'^2}}{U_r} + \frac{\frac{\partial^2 U_z}{\partial z'^2}}{U_z} = \nu \tag{17}$$

One side of this equation is a function of t' only, while the other is a function of r' and z'. The only way this can be true is if both sides are equal to a constant, ν. Using this fact it is possible to solve for U_t. That solution is

$$U_t = \exp(\nu t') \tag{18}$$

This equation implies that $\nu < 0$ because the solution for $u(r',z',t')$ cannot increase exponentially with time. Now it is possible to take the part of equation (17) which is a function of r' and z' and rearrange it so that there is an equation which is a function of r' equal to a function of z' which again must be equal to a constant.

$$\frac{1}{r'}\frac{\frac{\partial U_r}{\partial r'}}{U_r} + \frac{\frac{\partial^2 U_r}{\partial r'^2}}{U_r} - \nu = -\frac{\frac{\partial^2 U_z}{\partial z'^2}}{U_z} = \sigma \tag{19}$$

Taking the z' equation it is possible to solve for U_z.

$$U_z = \sin(\sqrt{\sigma}z') \tag{20}$$

From the boundary conditions on the ends of the chamber, σ can be determined.

$$\sigma = \left(\frac{j\pi R^*}{H}\right)^2 \tag{21}$$

where H is the height of the chamber.

The solution of the remaining equation is U_r.

$$U_r = J_o(\lambda_i r') \tag{22}$$

where the λ_i are the zeros of $J_o(\lambda_i) = 0$. Combining all of these solution results in the complete solution results in

$$u(r',z',t') = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} A_{ij} J_o(\lambda_i r') \sin\left(\frac{j\pi R^*}{H} z'\right) \exp\left(-\left(\lambda_i^2 + \left(\frac{j\pi R^*}{H}\right)^2\right) t'\right) \tag{23}$$

Using the initial condition, A_{ij} can be found.

$$A_{ij} = \frac{\int_0^1 \int_0^L r' J_o(\lambda_i r') \sin\left(\frac{j\pi R^*}{H} z'\right) dz' dr'}{\int_0^1 \int_0^L r' J_o^2(\lambda_i r') \sin^2\left(\frac{j\pi R^*}{H} z'\right) dz' dr'}$$

$$= \frac{4(1 - (-1)^j)}{j\pi\lambda_i J_1(\lambda_i)}$$

where $L = H/R^*$.

Inner-Outer Expansion

Results of the solution given by equation (23) are that $u(r',z',t')$ is almost a constant for most of the chamber, indicating that coagulation is much more important as a removal mechanism for the bulk of the aerosol than is diffusive deposition. The fact that the higher order approximations are very difficult to solve indicates that the solution might be found using an inner-outer expansion technique. The inner-outer expansion technique is used on problems which have several regions in which the processes occurring are of different nature. The classical example of such a problem is a boundary layer problem such as illustrated here. In this technique a solution is found describing the dominant process in each region. The boundary conditions for the solution in one region are then modified by using the boundary conditions which were shown to exist in the adjacent region. These modifications are repeated until the boundary conditions for adjacent regions match each other.

For the outer expansion, diffusion can be ignored in equation (9). This leads to

$$\frac{\partial n'}{\partial t'} = -\gamma n'^2 \tag{25}$$

which is the well known equation for coagulation developed by Smoluchowski and presented in Fuchs [1]. The solution for this equation is

$$n'(t') = \frac{1}{1 + \gamma t'} \tag{26}$$

The inner expansion begins with the assumption that near the wall the only removal mechanism of any significance is diffusive deposition on the wall. It is further assumed that the particles are diffusing only along the x coordinate. These assumptions seem reasonable due to the extremely large gradient which exists at the walls of the chamber. Thus the equation describing the depletion of the aerosol near the wall is

$$\frac{\partial n'}{\partial t'} = \frac{\partial^2 n'}{\partial x'^2} \tag{27}$$

where x is the distance from the wall. Carslaw and Jaeger [8] give a solution to this equation.

$$n'(x',t') = \mathrm{erf}\left(\frac{x}{2\sqrt{t'}}\right) \tag{28}$$

This solution technique is presented as a possible alternative to the successive approximation technique presented earlier. However, the inner-outer expansion technique is a somewhat less desirable approach. For the inner-outer expansion technique it is necessary to solve two problems while for the successive approximation technique only one problem need be solved. Further, matching the two solutions repeatedly is likely to be a problem whose difficulty is comparable to that of solving for the higher order approximations in the successive approximation technique.

CHAPTER III

GRAVITY SOLUTION

Equation

A somewhat more difficult case is the solution of equation (12) in the presence of a gravitational field. A transformation is made which removes the sedimentation term. This transformation is due to Wilhelm [6] and is

$$u(r',z',t') = f(r',z',t')\exp\left(\frac{\beta}{2}z' - \frac{\beta^2}{4}t'\right) \tag{29}$$

This transformation yields

$$\frac{\partial f}{\partial t'} = \nabla^2 f - \varepsilon \exp\left(-\frac{\beta}{2}z' + \frac{\beta^2}{4}t'\right) \tag{30}$$

The boundary conditions then become $f(r',z',t') = 0$ at the wall and $f(r',z',0) = \exp(-\frac{\beta}{2}z')$.

Solution

Equation (30) is solved by separation of variables in the same manner as was equation (15), resulting in

$$f(r',z',t') = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} A_{ij} J_o(\lambda_i r')\sin\left(\frac{j\pi R^*}{H}z'\right)\exp\left(-\left(\lambda_i^2 + \left(\frac{j\pi R^*}{H}t'\right)^2\right)\right) \tag{31}$$

where

$$A_{ij} = \frac{\int_0^1 \int_0^L r' \exp(-\frac{\beta}{2} z') J_o(\lambda_i r') \sin(\frac{j\pi R^*}{H} z') dz' dr'}{\int_0^1 \int_0^L r' J_o^2(\lambda_i r') \sin^2(\frac{j\pi R^*}{H} z') dz' dr'}$$

$$= \frac{4j\pi(1 - (-1)^j \exp(-\frac{\beta}{2}L))}{\lambda_i J_1(\lambda_i)(\frac{\beta^2 L^2}{4} + j^2\pi^2)} \qquad (32)$$

Solution Near the Wall

There are several areas in which this solution has difficulties. An examination of equation (29) will show where these difficulties occur. Values for β range from 3.58 X 10^{-3} for small particles to 1.11 X 10^{12} for large particles. Thus for certain particle sizes, the transformation given by equation (29) becomes so large that the results are meaningless. The solution does work for particles smaller than 0.04 micrometers where sedimentation is much less important that diffusion, and for particles larger than 0.7 micrometers where diffusion is much less important than sedimentation and for long times when sedimentation has essentially depleted the chamber.

Results from the zero-gravity solution indicate that the effects of diffusive deposition are limited to a thin boundary layer. Thus diffusive deposition has a negligible effect on the concentration of the bulk of the chamber and it seems reasonable to expect that the problems of the above solution can be overcome by ignoring diffusion altogether. This leads to the equation

$$\frac{\partial n'}{\partial t'} = - \beta\frac{\partial n'}{\partial z'} - \gamma n'^2 \qquad (33)$$

now applying the transformation in equation (11) the result is

$$\frac{\partial u}{\partial t'} = -\beta\frac{\partial u}{\partial z'} \tag{34}$$

The solution to this is in terms of a unit step function, s(x). The unit step function is defined as follows

$$s(x) = \begin{cases} 0 & x < 0 \\ 1 & x > 0 \end{cases}$$

So the solution to equation (34) is

$$u(r',z',t') = s\left(\frac{H}{R*} - z' - \beta t'\right) \tag{35}$$

This solution can be combined with the inner expansion solution of equation (28) to give the solution for the entire chamber.

CHAPTER IV

RESULTS AND DISCUSSION

Zero-Gravity

Figure 1 gives the results of the settling velocity calculations for unit density spheres in air at 23C and 1 atmosphere.

Figures 2 - 5 give the results of equation (23) which describes the depletion of a confined aerosol which is acted on only by coagulation and diffusive deposition. The first two figures give the concentration as a function of particle size for a location near the center of the chamber and times of 1 and 2 hours. These figures do not show any effects of diffusive deposition on the aerosol concentration and are therefore identical to a curve for coagulation alone. Figures 4 and 5 give similar information but for a location near the wall of the chamber. The dotted lines on the curves for the smaller particles show what the concentration would be if only coagulation were acting on the aerosol at that point. Thus it can be seen that diffusive deposition is not very effective as a removal mechanism for the bulk of the chamber. Near the wall, however, the situation is reversed. There is a steep gradient in concentration which drives diffusive deposition. Thus for a thin boundary layer the dominant removal mechanism is diffusive deposition. The steep gradient near the wall will reduce equation (14) to a one dimensional equation except at the corners. The solution to

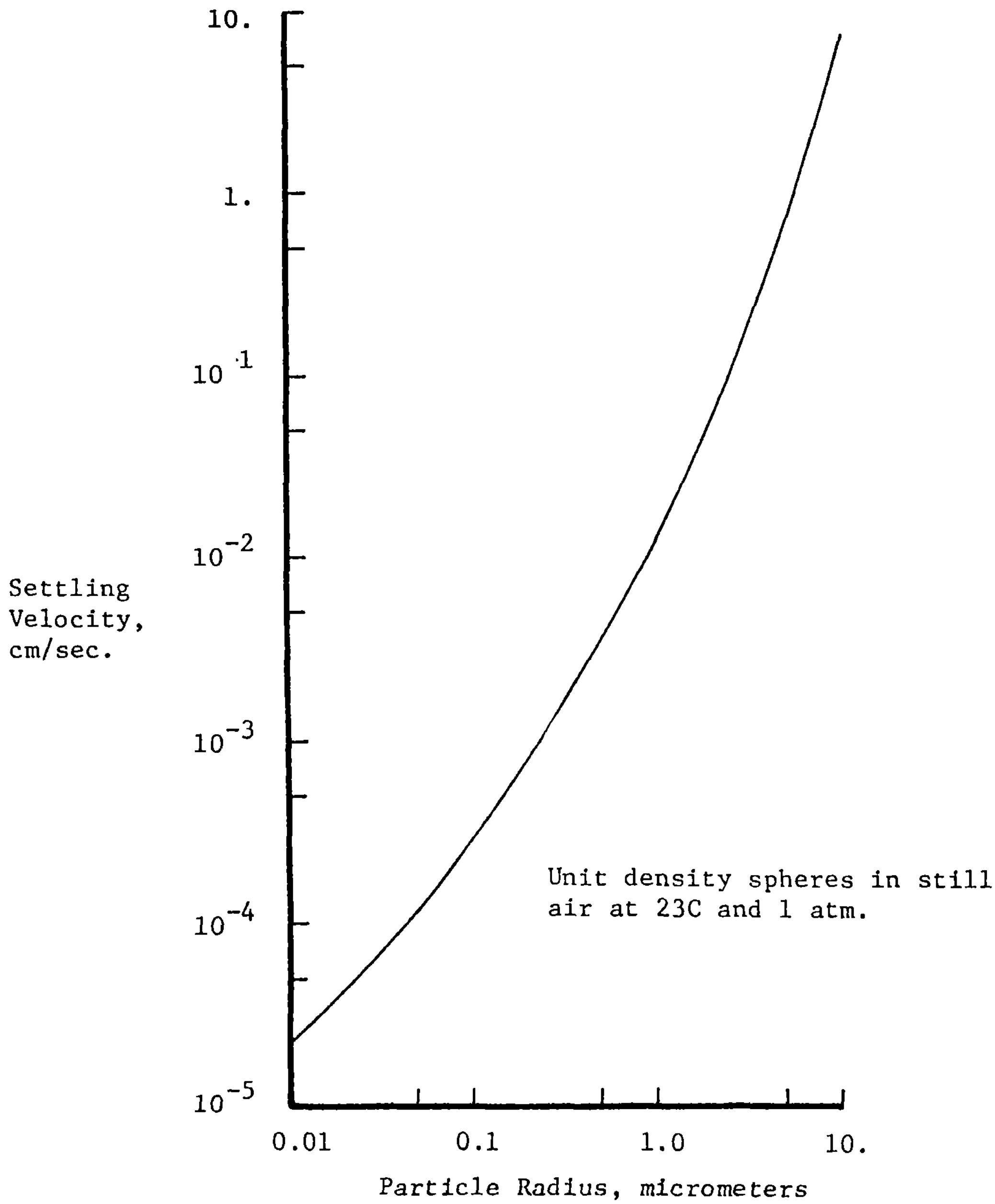

Figure 1. PARTICLE SETTLING VELOCITY.

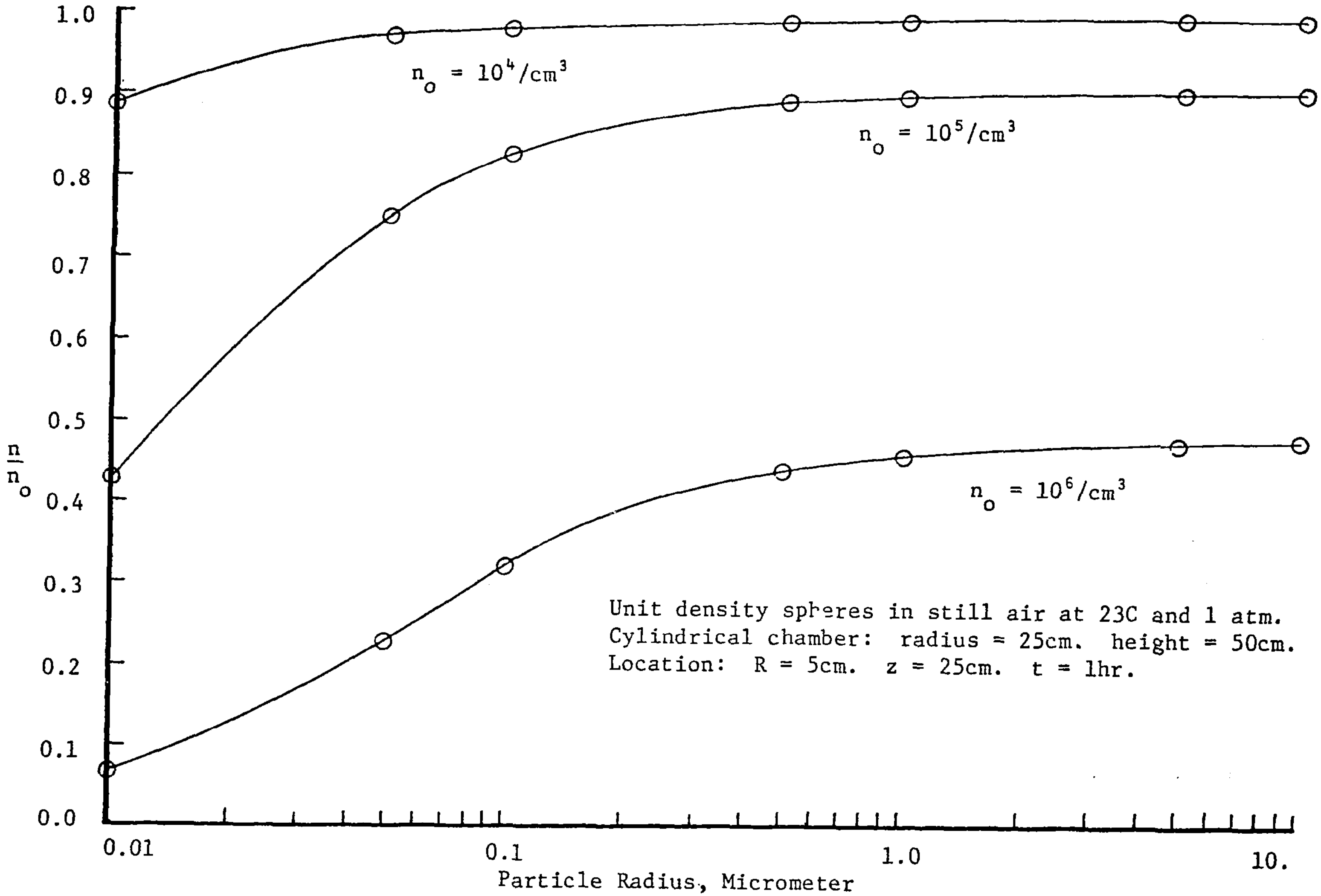

Figure 2. PARTICLE DEPLETION IN THE ABSENCE OF GRAVITY: IMPORTANCE OF COAGULATION.

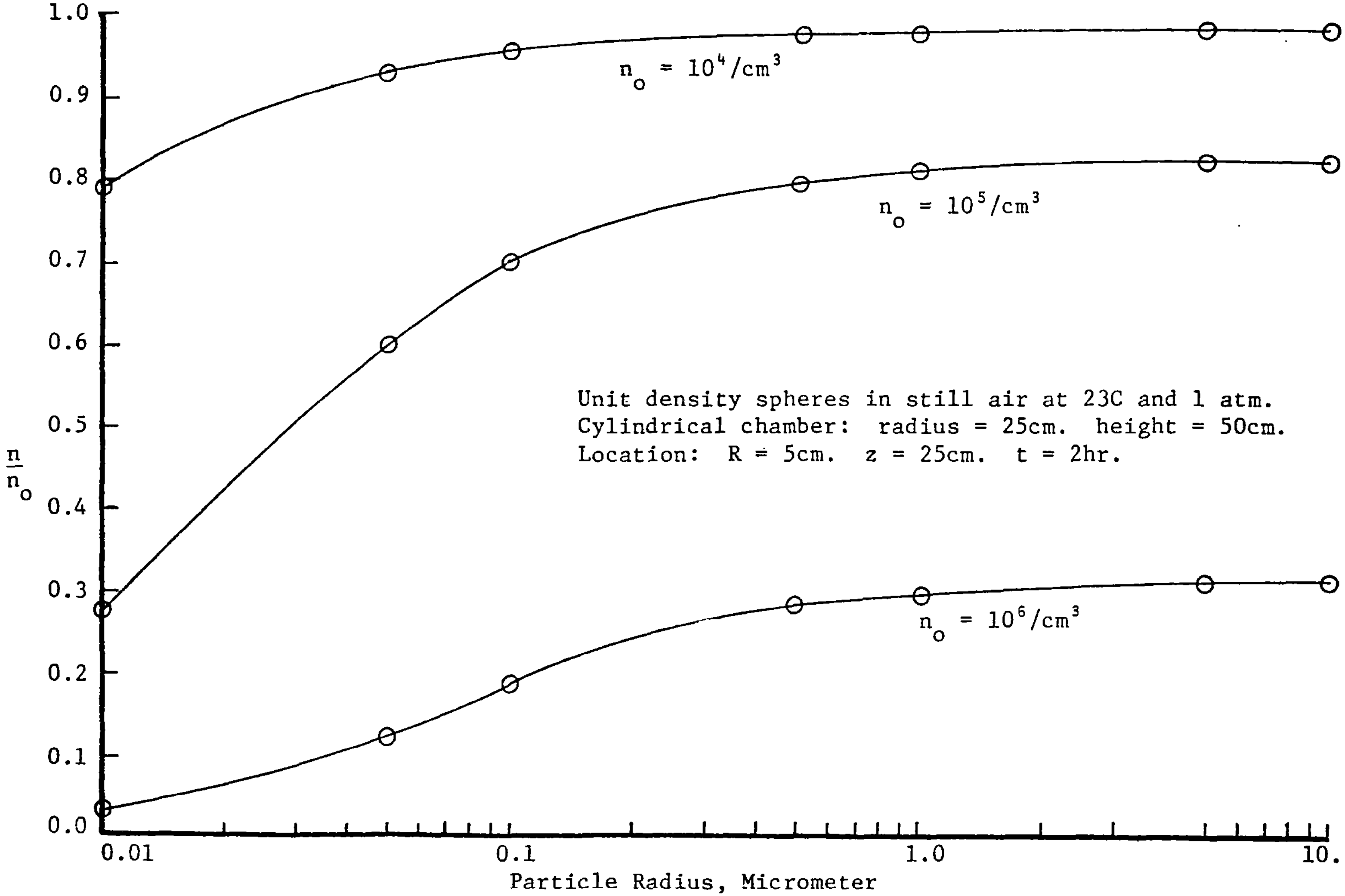

Figure 3. PARTICLE DEPLETION IN THE ABSENCE OF GRAVITY: IMPORTANCE OF COAGULATION.

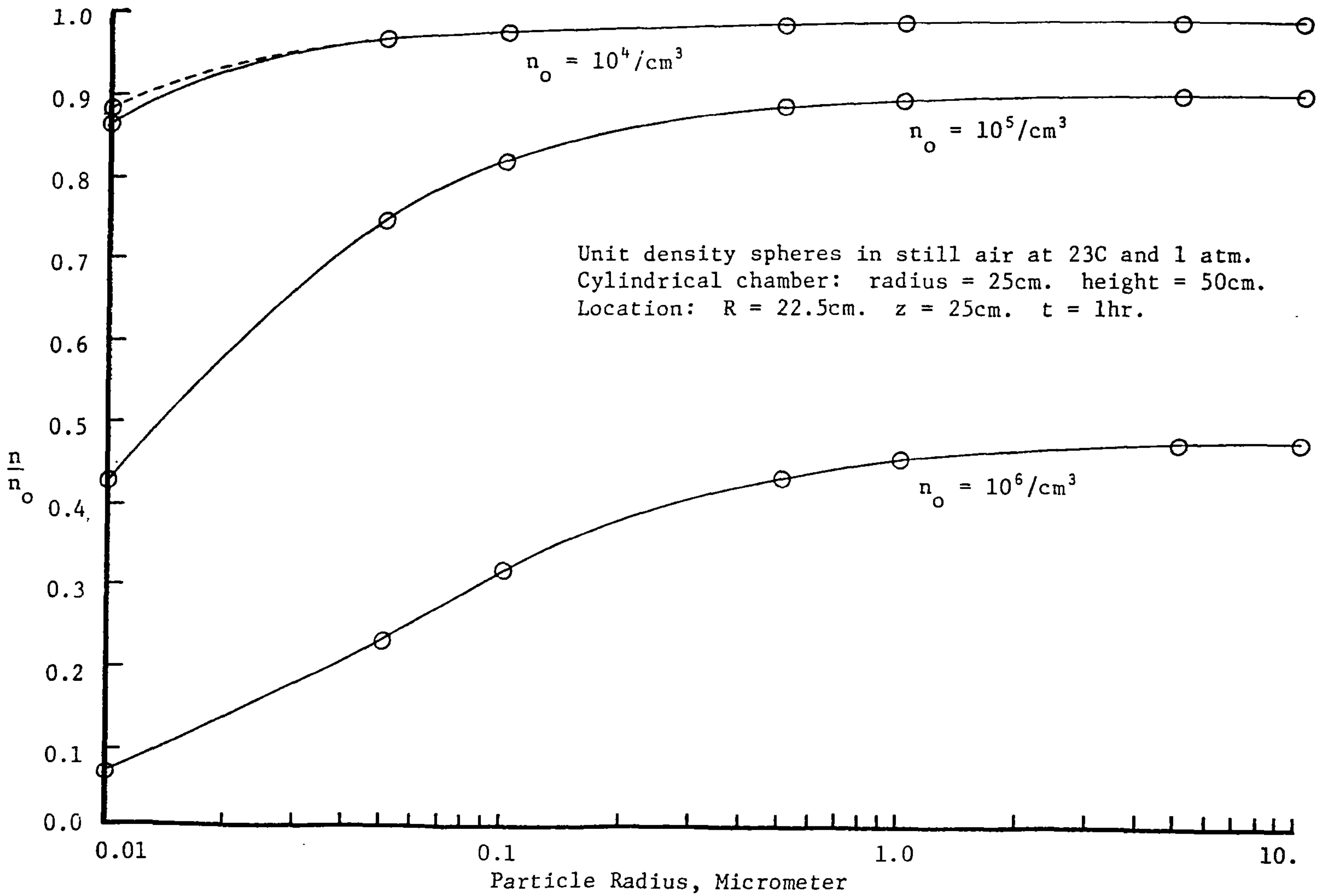

Figure 4. PARTICLE DEPLETION IN THE ABSENCE OF GRAVITY: IMPORTANCE OF COAGULATION.

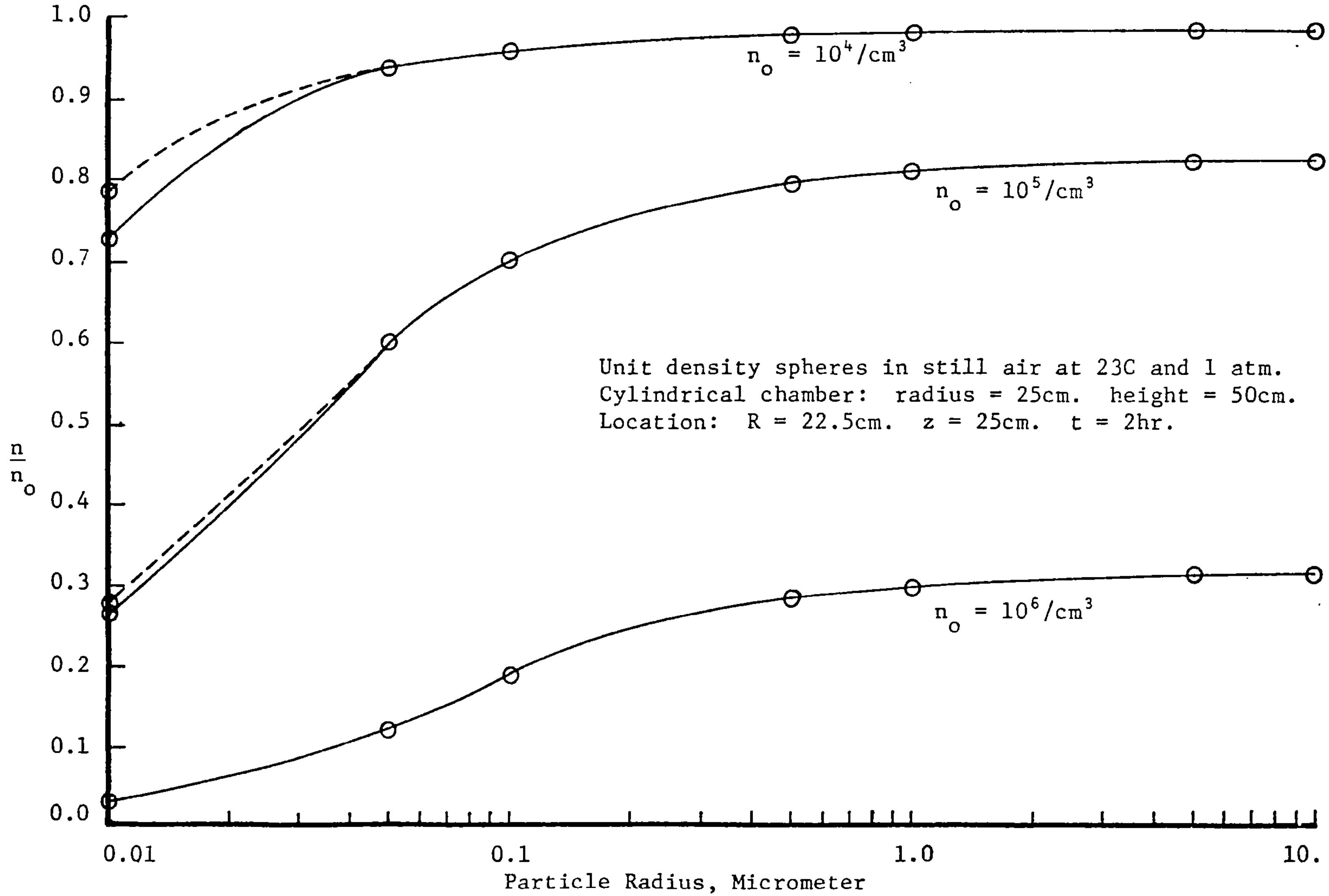

Figure 5. PARTICLE DEPLETION IN THE ABSENCE OF GRAVITY: IMPORTANCE OF COAGULATION.

the one dimensional diffusion equation (28). Figures 6 and 7 are concentration profiles for the region near the wall of the chamber and show the extent of the action of diffusive deposition for times of 1 and 2 hours respectively. Thus for the zeroth approximation, equation (15) gives the concentration for the entire chamber.

The zeroth approximation is sufficiently accurate for all but the most demanding applications. The higher order solutions are very difficult to obtain and contain only a small correction to the solution given by equation (23). Table I gives the values of the terms of equation (14) for various locations within the chamber and times of 1 and 2 hours. The values for locations near the center of the chamber are large relative to the other terms in equation (14) but are quite small. The size of ε for these locations is a further indication that there are no gradients and thus diffusive deposition is not important. The values are so large because of truncation error in evaluating equation (23) and not any fluctuations in aerosol concentration at those points. If the truncation error were not present it is expected that the value of ε would be zero. Substituting $\varepsilon = 0$ into equation (14) for the first approximation would yield exactly the same result as the zeroth approximation. Thus for those situations where $\varepsilon = 0$ the zeroth approxiamtion is exact.

The inner-outer expansion solution embodied in equations (25) through (28) give further evidence that the zeroth approximation is accurate because this solution technique gives the same results as those of equation (15). That one dimensional diffusion is the dominant removal mechanism near the wall is also shown by the fact that the solution to equation (27) predicted the difference between the curves for

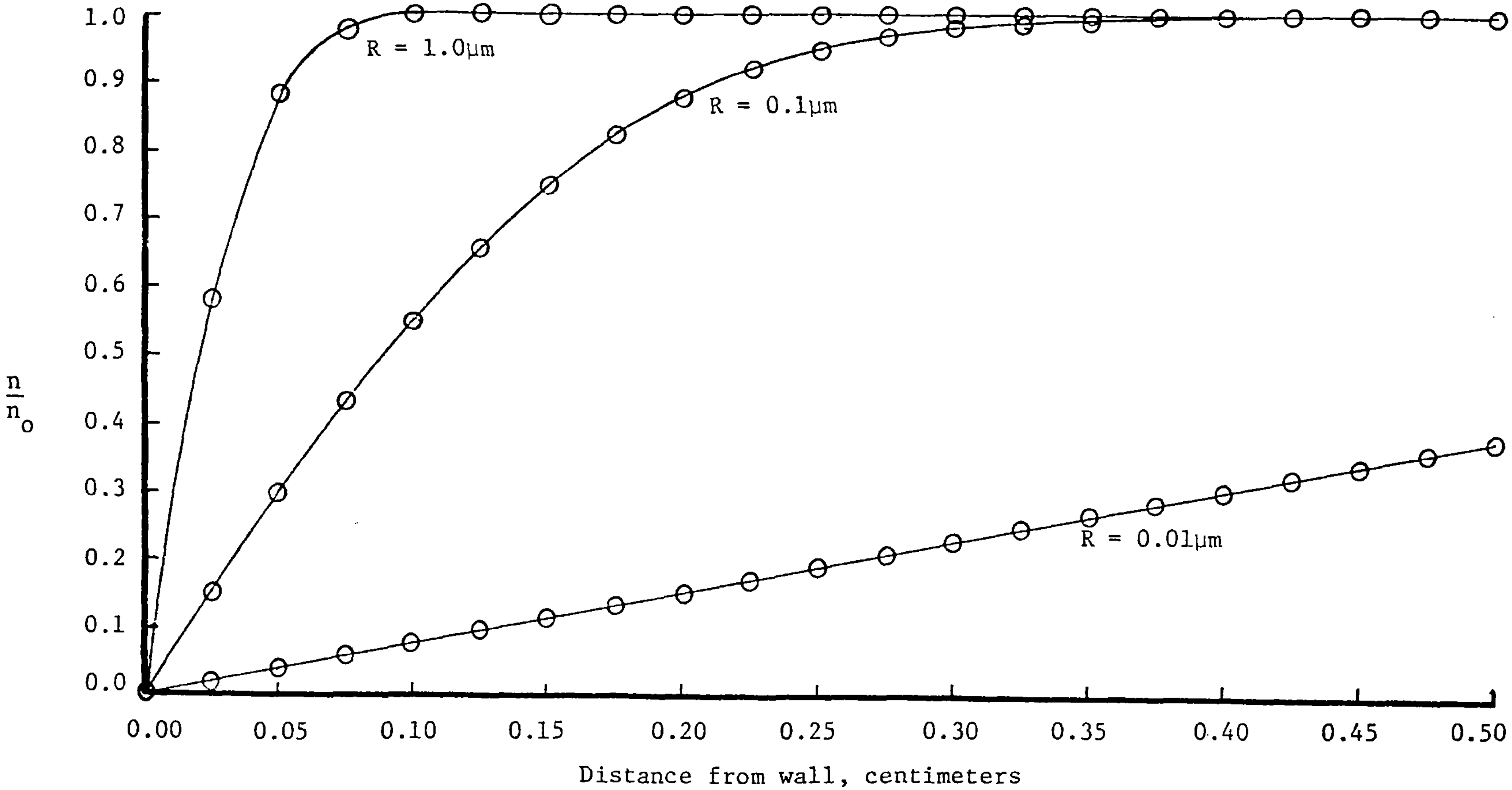

Figure 6. PARTICLE CONCENTRATION NEAR WALL DUE TO DIFFUSION ALONE.

Unit density shperes in still air at 23C and 1 atm.
Cylindrical chamber: radius = 25cm. height = 50cm.
Location: z = 25cm. t = 1hr.

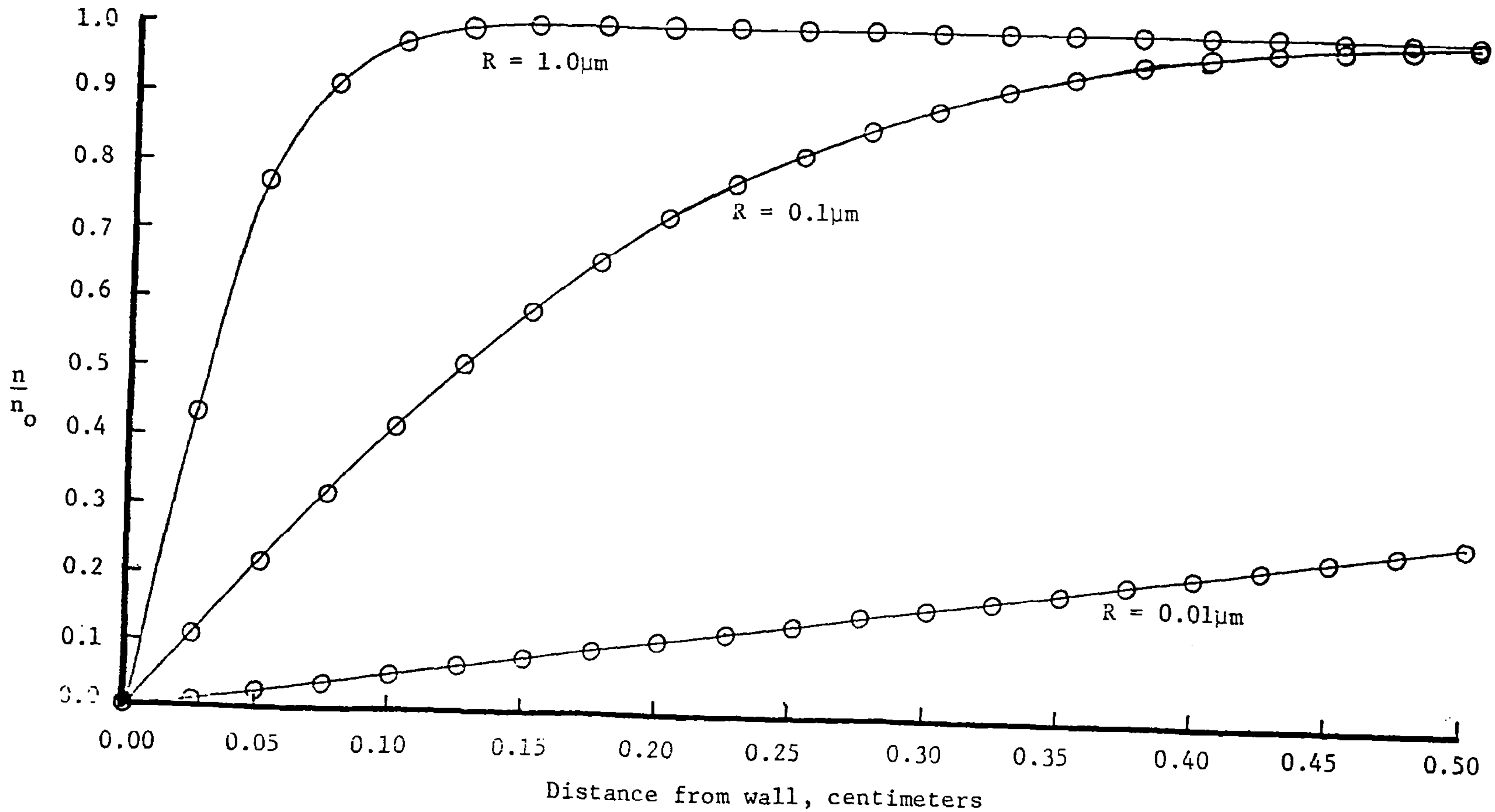

Figure 7. PARTICLE CONCENTRATION NEAR WALL DUE TO DIFFUSION ALONE.

Unit density shperes in still air at 23C and 1 atm.
Cylindrical chamber: radius = 25cm. height = 50cm.
Location: z = 25cm. t = 2hr.

Table I

VALUES OF TERMS IN EQUATION (14)

R(cm)	r(cm)	t(hr)	$\frac{\partial u}{\partial t'}$	$\nabla^2 u$	ε
1E-6	5	1	0.	3.05E-6	3.05E-6
1E-6	22.5	1	18.96	18.97	5.80E-3
1E-6	5	2	0.	4.18E-16	4.18E-16
1E-6	22.5	2	87.69	88.03	0.340
1E-5	5	1	0.	4.09E-9	4.09E-9
1E-5	22.5	1	0.	4.09E-9	4.09E-9
1E-5	5	2	0.	2.26E-12	2.26E-12
1E-5	22.5	2	0.	2.26E-12	2.26E-12
1E-4	5	1	0.	5.18E-6	5.18E-6
1E-4	22.5	1	0.	5.40E-6	5.40E-6
1E-4	5	2	0.	6.47E-6	6.47E-6
1E-4	22.5	2	0.	6.48E-6	6.48E-6
1E-3	5	1	0.	7.46E-6	7.46E-6
1E-3	22.5	1	0.	1.35E-5	1.35E-5
1E-3	5	2	0.	1.41E-5	1.41E-5
1E-3	22.5	2	0.	2.24E-5	2.24E-5

coagulation alone, depicted by the dotted lines, and the curves for both coagulation and diffusive deposition in figures 4 and 5 to within 1%.

Table I shows that the values for ε for locations near the wall are quite large relative to those far from the wall. Comparison with the values of the other terms in equation (14) shows that they are negligible. Thus the approximation calculated by ignoring ε for those regions was good.

Gravity

Equation (33) is the model of a confined aerosol which is acted on by sedimentation as well as coagulation and diffusive deposition. Figures 8 and 9 give the results of this model. Figures 8 and 9 are graphs of the concentration as a function of particle size for a location near the bottom of the chamber. An inportant result of this model is the sharp gradient which appears in the vertical extent of the chamber as a result of the action of gravity. This gradient moves downward with a velocity equal to the terminal settling velocity of the particles. Above the line of the gradient there are no particles. Below the line the concentration changes as if the particles were being acted on by coagulation and diffusive deposition.

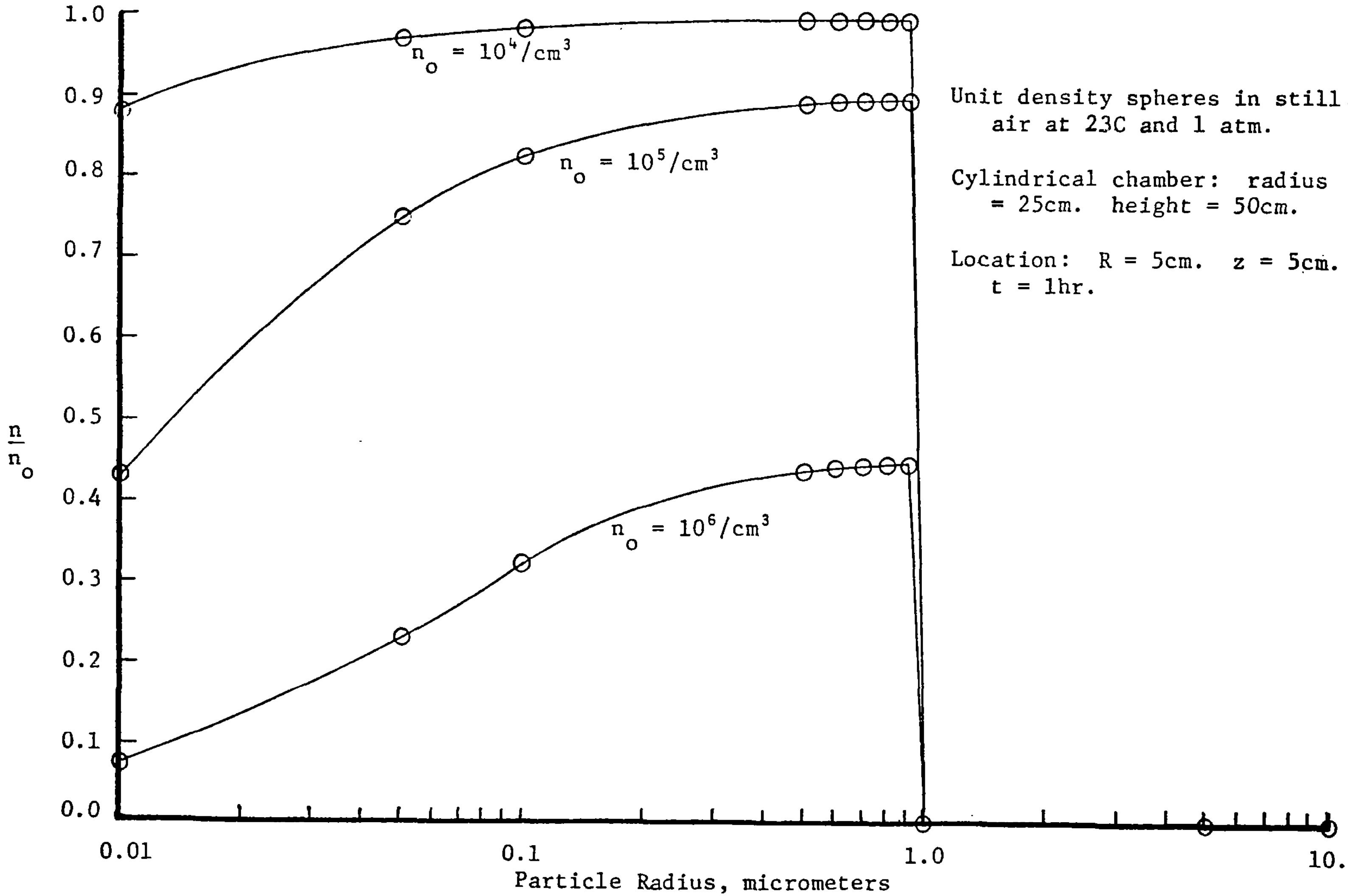

Figure 8. PARTICLE DEPLETION IN THE PRESENCE OF GRAVITY AND COAGULATION.

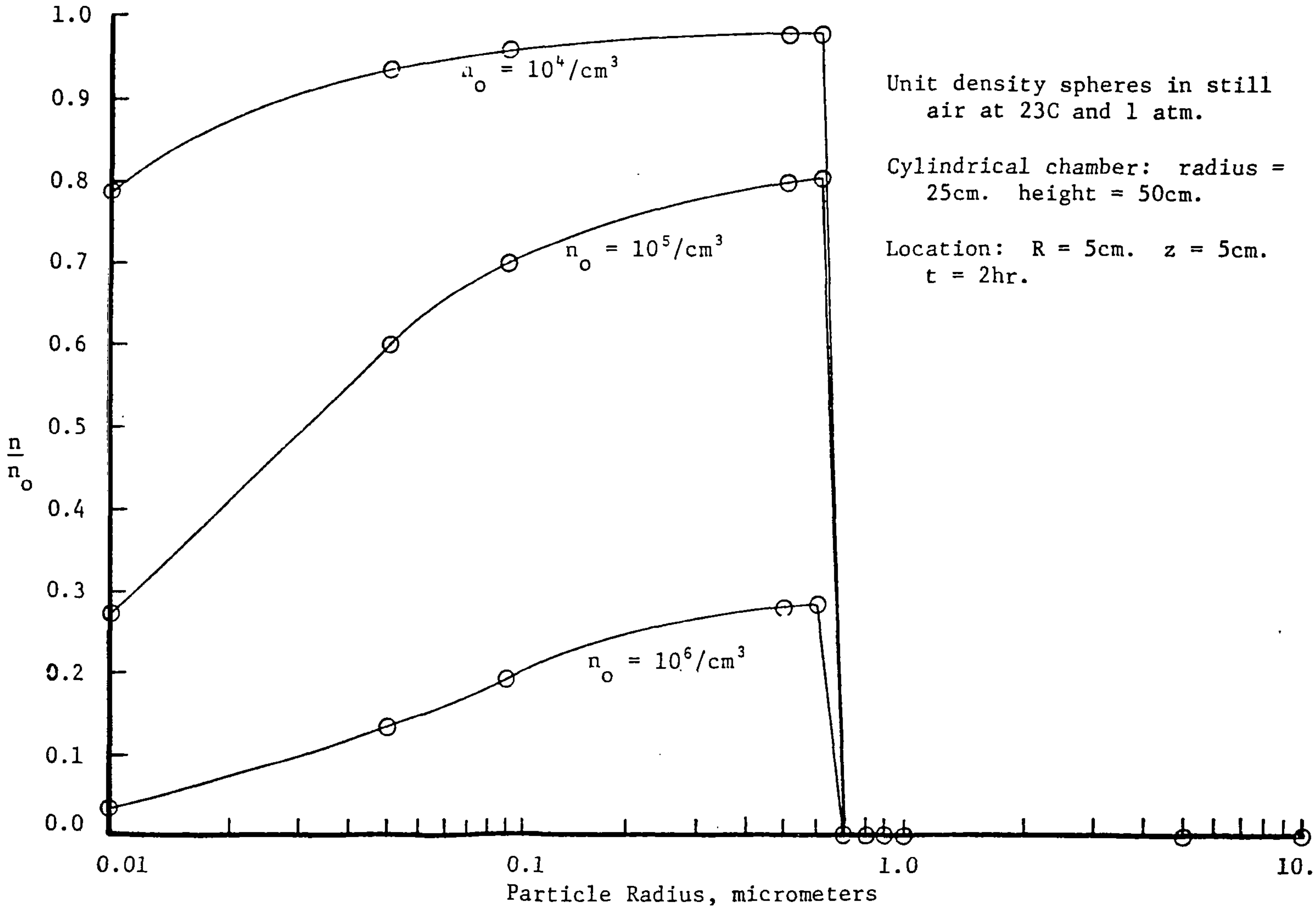

Figure 9. PARTICLE DEPLETION IN THE PRESENCE OF GRAVITY AND COAGULATION.

CHAPTER V

CONCLUSIONS

The aerosol depletion model given by equation (14) represents the action of a confined aerosol both in the presence and absence of gravity for the entire chamber. It was found that in the presence of a gravitational field, sedimentation was the dominant mechanism, even for small particles. When there is no gravitational field, coagulation is the most significant mechanism for removing particles from the bulk of the chamber.

An advantage of the zero-gravity model is that it embodies the solution for the entire chamber. The more conventional technique of inner-outer expansions requires that two different problems be solved and the solutions then matched. The matching problem is likely to present difficulties comparable to those of solving for the higher order approximations.

The results presented are those of the zeroth approximation. However, the higher order approximations would only yield a small correction to the zeroth approximation and thus may not be worthwhile in most cases.

The situation in the presence of gravity yields an important result in the sharp boundary which moves downward through the chamber. This result is not unreasonable and is substantiated by the results of the one dimensional diffusion work. This work indicated that aerosol particles do not diffuse very far from the location of the gradient which drives the diffusion. Nonetheless, diffusion is present and the boundary would be more or less blurred by it.

The model is not complete in that it does not directly deal with the shifting size distribution of particles caused by coagulation. Fuchs [1] indicates that there has been no significant time dependence in the coagulation coefficient detected in the terrestrial experiments done to date. This is because the expected increase in the coagulation coefficient due to the increased particle size is almost exactly offset by the decrease in diffusivity of the larger particle. The diffusion coefficient for the new particle would be less, but this would have the effect of decreasing the effect of diffusive deposition on the particle concentration. Thus this effect should not require a major correction. The terminal settling velocity of the new particles would be greater and this could cause a problem for the gravity model. It is expected that for the lower initial concentrations and short times that the results of the gravity model would be valid because there would only be a few of these larger particles formed. An attempt to deal with this problem would follow the lines of research presented by Tolfo [9]. This would involve writing a model such as this for each size class and solving them simultaneously. Some further work that would be instructive would be to find the higher order approximations, although it is expected that they will not provide much additional information.

There is much experimental work that needs to be done. Data are needed to validate this model. These data should take the form of aerosol concentrations for various times and locations within the chamber, both in the presence and absence of gravity. The values of the coagulation coefficient and diffusion coefficient used in this model were theoretical. A zero-gravity experiment would be instrumental in obtaining measurements of these quantities. These measurements are severely hampered in terrestrial experiments by the action of gravity. Zero-gravity experiments could be designed which would provide direct measurements of these quantities, thus validating that portion of this model and advancing our knowledge of aerosol science.

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[9] Tolfo, Flavio, J. Aerosol Sci., 8, 9-19, 1977.

APPENDIX A

```
      PROGRAM SOLUTN (INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
C
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C         PROGRAM CALCULATES THE ZEROTH APPROXIMATION TO THE SOLUTION
C         OF THE AEROSOL DECAY EQUATION FOR A ZERO GRAVITY ENVIRONMENT
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C         IN THIS PART VARIABLES ARE INITIALIZED AND PROGRAM OPERATION
C         IS CONTROLLED
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C
      DIMENSION F(11,11),U(11,11),EPSLON(11,11),Z(11),CONCN(11,11),
     1 SERSIN(11),DUDZ(11,11),DUDR(11,11),SERJ0(11)
      COMMON/ZZ/BETA,PI,PI02,PI02SQ,BTASQ,EXPBTA
      COMMON/RR/TIME
C
C * * * * * * INITIALIZE
C
      TIMPRM=3600.
      CHMRAD=25.
      CHMHT=50.
      CONCI=1.E4
      IR=11
      IZ=11
      RINC=.1
      ZINC=.2
      PI=4.*ATAN(1.)
      PI02=PI/2.
      PI02SQ=PI02*PI02
      ITERMZ=350
      ITERMR=500
   10 CONTINUE
      IPASS=1
      READ (5,20) R,V,COAG,D
   20 FORMAT (4F10.0)
      IF (EOF(5)) 270,30,270
   30 CONTINUE
      WRITE (6,40) R,V,D,COAG,TIMPRM,CONCI
   40 FORMAT (1H1,//,10X, 18HTHIS OUTPUT IS FOR,//,15X, 13HPARTICLE SIZE
     1,15X,1PE8.1,/,15X, 17HSETTLING VELOCITY,11X,1PE11.4,/,15X, 21HDIFF
     2USION COEFFICIENT,7X,1PE11.4,/,15X, 23HCOAGULATION COEFFICIENT,5X,
     31PE11.4,/,15X,  4HTIME,24X,0PF8.1,/,15X, 21HINITIAL CONCENTRATION,
     47X,1PE8.1,//)
      BETA=CHMRAD*V/D
      GAMMA=CHMRAD*CHMRAD*COAG*CONCI/D
      TIME=TIMPRM*D/(CHMRAD*CHMRAD)
      BTASQ=BETA*BETA/4.
      BTAOV2=BETA/2.
      EXPBTA=EXP(-BETA*CHMHT/(2.*CHMRAD))
      BTATIM=BTASQ*TIME
      XPTIME=EXP(BTATIM)
      GMATIM=GAMMA*TIME
      TOGMAT=2.*GMATIM
C
C * * * * * * SUM SERIES FOR Z
C
      Z(1)=0.
      DO 50 I=2,IZ
         Z(I)=Z(I-1)+ZINC
   50 CONTINUE
      DO 60 I=1,IZ
         CALL SINES (Z(I),SERSIN(I),ITERMZ)
   60 CONTINUE
C
C * * * * * * SUM SERIES FOR R
C
      RAD=0.
      DO 70 I=1,IR
         CALL BESSEL (RAD,SERJ0(I),ITERMR)
         RAD=RAD+RINC
   70 CONTINUE
C
C * * * * * * CALCULATE TOTAL SOLUTION
```

```
C
      DO 110 I=1,IR
         DO 100 J=1,IZ
            F(I,J)=SERJ0(I)*SERSIN(J)
            XEXP=BTAOV2*Z(J)-BTATIM
            IF (XEXP.GT.600.) GO TO 80
            U(I,J)=F(I,J)*EXP(XEXP)
            CONCN(I,J)=U(I,J)/(1.+GMATIM*U(I,J))
            GO TO 100
   80       CONTINUE
            WRITE (6,90) I,J,F(I,J),XEXP
   90 FORMAT (15X,  4HI = ,I3,3X,  4HJ = ,I3,3X,  9HF(I,J) = ,1PE11.4,3X
     1,  7HXEXP = ,1PE11.4)
            IPASS=-1
  100    CONTINUE
  110 CONTINUE
      IF (IPASS.LT.0) GO TO 200
C
C * * * * * * CALCULATE DERIVATIVES FOR EPSILON
C
      DO 120 I=1,IR
         DUDR(1,I)=(U(1,I)-U(2,I))/(-RINC)
  120 CONTINUE
      DO 140 I=2,IR
         DO 130 J=1,IZ
            DUDR(I,J)=(U(I-1,J)-U(I,J))/(-RINC)
  130    CONTINUE
  140 CONTINUE
      DO 150 I=1,IZ
         DUDZ(I,1)=(U(I,1)-U(I,2))/(-ZINC)
  150 CONTINUE
      DO 170 I=1,IR
         DO 160 J=2,IZ
            DUDZ(I,J)=(U(I,J-1)-U(I,J))/(-ZINC)
  160    CONTINUE
  170 CONTINUE
C
C * * * * * * CALCULATE EPSILON
C
      DO 190 I=1,IR
         DO 180 J=1,IZ
            EPSLON(I,J)=(TOGMAT/(1.+GMATIM*U(I,J)))*(DUDR(I,J)*DUDR(I,J)
     1      +DUDZ(I,J)*DUDZ(I,J))
  180    CONTINUE
  190 CONTINUE
C
C * * * * * * OUTPUT VARIABLES
C
  200 CONTINUE
      WRITE (6,210)
  210 FORMAT (15X,  5HCONCN)
      CALL TERMS (IR,IZ,CONCN)
      WRITE (6,220)
  220 FORMAT (15X,  7HEPSILON)
      CALL TERMS (IR,IZ,EPSLON)
      WRITE (6,230)
  230 FORMAT (15X,  1HU)
      CALL TERMS (IR,IZ,U)
      WRITE (6,240)
  240 FORMAT (15X,  4HDUDR)
      CALL TERMS (IR,IZ,DUDR)
      WRITE (6,250)
  250 FORMAT (15X,  4HDUDZ)
      CALL TERMS (IR,IZ,DUDZ)
      WRITE (6,260)
  260 FORMAT (15X,  1HF)
      CALL TERMS (IR,IZ,F)
      GO TO 10
  270 CONTINUE
      STOP
C
      END
```

```
      SUBROUTINE BESSL (GNU,X,BESSEL)
C
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C        THIS SR CALCULATES THE BESSEL FUNCTION, J(X), OF ORDER GNU
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C
      DATA AA21/.25/,AA41/-.375/,AA42/.15625/,AA61/1.875/,
     1 AA62/-1.15625/,AA63/.1171875/,AA81/-19.6875/,AA82/14.2265625/,
     2 AA83/-2.38671875/,AA84/.0952148437/,AA101/354.375/,
     3 AA102/-277.875/,AA103/58.22460938/,AA104/-4.100585938/,
     4 AA105/.0809326171/,BB21/.5/,BB41/-.25/,BB42/.041666666666/,
     5 BB61/.75/,BB62/-.35/,BB63/.0125/,BB81/-5.625/,BB82/3.6026788571/,
     6 BB83/-.4241071429/,BB84/5.580357143/,BB101/78.75/,BB102/-58./,
     7 BB103/10.28645833/,BB104/-.347222222222/,BB105/3.038194444E-3/
C
C * * * * * * INITIALIZE
C
      PI=4.*ATAN(1.)
      PI02=PI/2.
      ALPHA=GNU*GNU-.25
      T=1./X
      TSQ=T*T
C
C * * * * * * CALCULATE COEFFICIENTS
C
      A2=ALPHA*AA21
      A4=(AA42*ALPHA+AA41)*ALPHA
      A6=((AA63*ALPHA+AA62)*ALPHA+AA61)*ALPHA
      A8=(((AA84*ALPHA+AA83)*ALPHA+AA82)*ALPHA+AA81)*ALPHA
      A10=((((AA105*ALPHA+AA104)*ALPHA+AA103)*ALPHA+AA102)*ALPHA+AA101)*
     1ALPHA
      B2=BB21*ALPHA
      B4=(BB42*ALPHA+BB41)*ALPHA
      B6=((BB63*ALPHA+BB62)*ALPHA+BB61)*ALPHA
      B8=(((BB84*ALPHA+BB83)*ALPHA+BB82)*ALPHA+BB81)*ALPHA
      B10=((((BB105*ALPHA+BB104)*ALPHA+BB103)*ALPHA+BB102)*ALPHA+BB101)*
     1ALPHA
C
C * * * * * * CALCULATE INTERMEDIATE FUNCTIONS
C
      B=((((A10*TSQ+A8)*TSQ+A6)*TSQ+A4)*TSQ+A2)*TSQ+1.
      PRTPHI=((((B10*TSQ+B8)*TSQ+B6)*TSQ+B4)*TSQ+B2)*TSQ+1.
      PHI=PRTPHI/T-(GNU+.5)*PI02
C
C * * * * * * CALCULATE BESSEL FUNCTION
C
      BESSEL=B*SQRT(T/PI02)*COS(PHI)
      RETURN
C
      END
```

```
      SUBROUTINE BLAMDA (XLAMDA,ITERM)
C
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C        FINDS THE FIRST ITERM ROOTS OF THE ZERO ORDER BESSEL FTN
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C
      DIMENSION XLAMDA(ITERM)
C
C ****** INITIALIZE
C
      PI=4.*ATAN(1.)
      A=2.4
      ERROR=1.E-8
      DO 60 I=1,ITERM
         B=A+1.
         X=B
         IF (A.LE.10.) CALL BESJ (A,0,XJOFA,1.E-6,IER)
         IF (B.LE.10.) CALL BESJ (B,0,XJOFB,1.E-6,IER)
         IF (A.GT.10.) CALL BESSL (0.,A,XJOFA)
         IF (B.GT.10.) CALL BESSL (0.,B,XJOFB)
   10    CONTINUE
         IF (X.GT.10.) CALL BESSL (0.,X,XJOFX)
         IF (X.LE.10.) CALL BESJ (X,0,XJOFX,1.E-6,IER)
         IF (XJOFA*XJOFX) 20,50,30
   20    CONTINUE
         B=X
         XJOFB=XJOFX
         GO TO 40
   30    CONTINUE
         A=X
         XJOFA=XJOFX
   40    CONTINUE
         IF (ABS(XJOFX).LE.ERROR) GO TO 50
         X=(A*XJOFB-B*XJOFA)/(XJOFB-XJOFA)
         GO TO 10
   50    CONTINUE
         A=X+3.
         XLAMDA(I)=X
   60 CONTINUE
      RETURN
C
      END
```

```
      SUBROUTINE SINES (Z,F,ITERM)
C
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C        THIS SR CALCULATES THE SIN SERIES, F, FOR POSITION Z
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C
      DIMENSION A(350   ),SINE(350   ),TERM(350   )
      COMMON/RR/TIME
      COMMON/ZZ/BETA,PI,PIO2,PIO2SQ,BTASQ,EXPBTA
      F=0.
      XMN1=1.
      DO 10 ITRM=1,ITERM
         XMN1=XMN1*(-1.)
         XTRM=FLOAT(ITRM)
         EXPTIM=EXP(-XTRM*XTRM*PIO2SQ*TIME)
         ARG=XTRM*PIO2*Z
         A(ITRM)=XTRM*PIO2*(1.-XMN1*EXPBTA)/(BTASQ+XTRM*XTRM*PIO2SQ)
         SINE(ITRM)=SIN(ARG)
         TERM(ITRM)=A(ITRM)*SINE(ITRM)*EXPTIM
         F=F+TERM(ITRM)
   10 CONTINUE
      RETURN
C
      END
```

```
      SUBROUTINE BESSEL (R,F,ITERM)
C
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C        THIS SR CALCULATES THE J0 SERIES, F, FOR POSITION R
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C
      DIMENSION XLMDA(500  ),BESSL1(500  ),BESSL0(500  ),TERM(500  ),
     1 A(500  )
      COMMON/RR/TIME
      F=0.
      ERROR=1.E-6
      CALL BLAMDA (XLMDA,ITERM)
      DO 80 ITRM=1,ITERM
         IF (XLMDA(ITRM).GT.10.) GO TO 20
         CALL BESJ (XLMDA(ITRM),1,BESSL1(ITRM),ERROR,IER)
         IF (IER.NE.0) WRITE (6,10) IER,XLMDA(ITRM),BESSL1(ITRM)
   10 FORMAT (10X,  5HIER= ,I3,  9H LAMDA = ,1PE11.4,  6H J1 = ,1PE11.4)
         GO TO 30
   20    CONTINUE
         CALL BESSL (1.,XLMDA(ITRM),BESSL1(ITRM))
   30    CONTINUE
         ARG=R*XLMDA(ITRM)
         IF (ARG.EQ.0.) GO TO 60
         IF (ARG.GT.10.) GO TO 50
         CALL BESJ (ARG,0,BESSL0(ITRM),ERROR,IER)
         IF (IER.NE.0) WRITE (6,40) IER,ARG,BESSL0(ITRM)
   40 FORMAT (10X,  6HIER = ,I3,  7H ARG = ,1PE11.4,  6H J0 = ,1PE11.4)
         GO TO 70
   50    CONTINUE
         CALL BESSL (0.,ARG,BESSL0(ITRM))
         GO TO 70
   60    CONTINUE
         BESSL0(ITRM)=1.
   70    CONTINUE
   80 CONTINUE
      DO 90 I=1,ITERM
         A(I)=2./(BESSL1(I)*XLMDA(I))
   90 CONTINUE
      DO 100 ITRM=1,ITERM
         EXPTIM=EXP(-XLMDA(ITRM)*XLMDA(ITRM)*TIME)
         TERM(ITRM)=A(ITRM)*BESSL0(ITRM)*EXPTIM
         F=F+TERM(ITRM)
  100 CONTINUE
      RETURN
C
      END
```

```
      SUBROUTINE TERMS (ITERM,JTERM,A)
      DIMENSION A(ITERM,JTERM)
      WRITE (6,10)
   10 FORMAT (/)
      DO 30 K=1,JTERM
         WRITE (6,20) (A(J,K),J=1,11)
   20 FORMAT (3X,11(1PE9.2,3X))
   30 CONTINUE
      IF (ITERM.LE.11) GO TO 70
      WRITE (6,10)
      DO 40 K=1,JTERM
         WRITE (6,20) (A(J,K),J=12,22)
   40 CONTINUE
      IF (ITERM.LE.22) GO TO 70
      WRITE (6,10)
      DO 50 K=1,JTERM
         WRITE (6,20) (A(J,K),J=23,33)
   50 CONTINUE
      IF (ITERM.LE.33) GO TO 70
      WRITE (6,10)
      DO 60 K=1,JTERM
         WRITE (6,20) (A(J,K),J=34,44)
   60 CONTINUE
   70 CONTINUE
      WRITE (6,80)
   80 FORMAT (//)
      RETURN
C
      END
```

APPENDIX B

```
      PROGRAM SOLUTN (INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
C
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C         PROGRAM CALCULATES THE ZEROTH APPROXIMATION TO THE SOLUTION
C         OF THE AEROSOL DECAY EQUATION FOR A GRAVITY ENVIRONMENT
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C         IN THIS PART VARIABLES ARE INITIALIZED AND PROGRAM OPERATION
C         IS CONTROLLED
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C
      DIMENSION F(11,11),U(11,11),EPSLON(11,11),Z(11),CONCN(11,11),
     1 SERSIN(11),DUDZ(11,11),DUDR(11,11),SERJ0(11)
      COMMON/ZZ/BETA,PI,PI02,PI02SQ,BTASQ,EXPBTA
      COMMON/RR/TIME
C
C * * * * * * INITIALIZE
C
      TIMPRM=7200.
      CONCI=1.E5
      CHMRAD=25.
      CHMHT=50.
      H=CHMHT/CHMRAD
      IR=11
      IZ=11
      RINC=.1
      ZINC=.2
      PI=4.*ATAN(1.)
      PI02=PI/2.
      PI02SQ=PI02*PI02
      ITERMZ=350
      ITERMR=500
      Z(1)=0.
      DO 10 I=2,IZ
         Z(I)=Z(I-1)+ZINC
   10 CONTINUE
   20 CONTINUE
      READ (5,30) R,V,COAG,D
   30 FORMAT (4F10.0)
      IF (EOF(5)) 210,40,210
   40 CONTINUE
      WRITE (6,50) R,V,D,COAG,TIMPRM,CONCI
   50 FORMAT (1H1,//,10X, 18HTHIS OUTPUT IS FOR,//,15X, 13HPARTICLE SIZE
     1,15X,1PE8.1,/,15X, 17HSETTLING VELOCITY,11X,1PE11.4,/,15X, 21HDIFF
     2USION COEFFICIENT,7X,1PE11.4,/,15X, 23HCOAGULATION COEFFICIENT,5X,
     31PE11.4,/,15X,  4HTIME,24X,0PF8.1,/,15X, 21HINITIAL CONCENTRATION,
     47X,1PE8.1,//)
      BETA=CHMRAD*V/D
      GAMMA=CHMRAD*CHMRAD*COAG*CONCI/D
      TIME=TIMPRM*D/(CHMRAD*CHMRAD)
      BTASQ=BETA*BETA/4.
      BTAOV2=BETA/2.
      EXPBTA=EXP(-BETA*CHMHT/(2.*CHMRAD))
      BTATIM=BTASQ*TIME
      BTTIME=BETA*TIME
      XPTIME=EXP(BTATIM)
      GMATIM=GAMMA*TIME
      TOGMAT=2.*GMATIM
C
C * * * * * * CALCULATE TOTAL SOLUTION
C
      DO 70 I=1,IR
         DO 60 J=1,IZ
            STPFN1=Z(J)-BTTIME
            STPFN2=STPFN1-H
            IF (STPFN1.LT.0.) SPFN1=0.
            IF (STPFN1.GE.0.) SPFN1=1.
            IF (STPFN2.LT.0.) SPFN2=0.
            IF (STPFN2.GE.0.) SPFN2=1.
            U(I,J)=SPFN1-SPFN2
            CONCN(I,J)=U(I,J)/(1.+GMATIM*U(I,J))
   60    CONTINUE
   70 CONTINUE
```

```
      DO 80 I=1,11
         U(I,11)=0.
         U(11,I)=0.
         CONCN(I,11)=0.
         CONCN(11,I)=0.
   80 CONTINUE
C
C * * * * * * CALCULATE DERIVATIVES FOR EPSILON
C
      DO 90 I=1,IR
         DUDR(1,I)=(U(1,I)-U(2,I))/(-RINC)
   90 CONTINUE
      DO 110 I=2,IR
         DO 100 J=1,IZ
            DUDR(I,J)=(U(I-1,J)-U(I,J))/(-RINC)
  100    CONTINUE
  110 CONTINUE
      DO 120 I=1,IZ
         DUDZ(I,1)=(U(I,1)-U(I,2))/(-ZINC)
  120 CONTINUE
      DO 140 I=1,IR
         DO 130 J=2,IZ
            DUDZ(I,J)=(U(I,J-1)-U(I,J))/(-ZINC)
  130    CONTINUE
  140 CONTINUE
C
C * * * * * * CALCULATE EPSILON
C
      DO 160 I=1,IR
         DO 150 J=1,IZ
            IF (ABS(DUDR(I,J)).GE.1.E270.OR.ABS(DUDZ(I,J)).GE.1.E270) GO
     1       TO 150
            EPSLON(I,J)=(TOGMAT/(1.+GMATIM*U(I,J)))*(DUDR(I,J)*DUDR(I,J)
     1      +DUDZ(I,J)*DUDZ(I,J))
  150    CONTINUE
  160 CONTINUE
C
C * * * * * * OUTPUT VARIABLES
C
      CALL TERMS (IR,IZ,CONCN)
      WRITE (6,170)
  170 FORMAT (15X,  7HEPSILON)
      CALL TERMS (IR,IZ,EPSLON)
      WRITE (6,180)
  180 FORMAT (15X,  1HU)
      CALL TERMS (IR,IZ,U)
      WRITE (6,190)
  190 FORMAT (15X,  4HDUDR)
      CALL TERMS (IR,IZ,DUDR)
      WRITE (6,200)
  200 FORMAT (15X,  4HDUDZ)
      CALL TERMS (IR,IZ,DUDZ)
      GO TO 20
  210 CONTINUE
      STOP
C
      END
```

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16. ABSTRACT

The feasibility and scientific benefits of a zero-gravity aerosol study in an orbiting laboratory have been examined. A macroscopic model was devised to deal with the simultaneous effects of diffusion and coagulation of particles in the confined aerosol. The particle depletion rate is given by a second-order, nonlinear partial differential equation. An analytical solution was found by treating the particle coagulation and diffusion constants as ensemble parameters and employing a transformation of variables. The solution was used to carry out simulated zero-gravity aerosol decay experiments in a compact cylindrical chamber. The results demonstrate that the limitations of physical space and time imposed by the orbital situation are not prohibitive in terms of observing the history of an aerosol confined under zero-gravity conditions.

While the absence of convective effects would be a definite benefit for the experiment, the mathematical complexity of the problem is not greatly reduced when the gravitational term drops out of the equation. Since the present model does not deal directly with the evolution of the particle size distribution, it may be desirable to develop more detailed models before undertaking an orbital experiment. Moreover, it was found that the accuracy of measurement required to validate various kinetic models may not be presently available for the full range of aerosol particle sizes and concentrations of interest.

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